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Quantum-chemical calculation of the adsorption energy of the Pb atom on the graphene

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Abstract

© 2018 Author(s). Graphene can be used as sensors to detect toxic heavy metals in peripheral blood. This requires a clear understanding of adsorption process on the graphene surface. The DFT-functional method is used to calculate adsorption energy. In the article we present the calculation results and analyse interaction of Pb atom with graphene surface. It is shown that the Pb atom in B-site position on a graphene plane has a minimum of energy.

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